Fig. 1

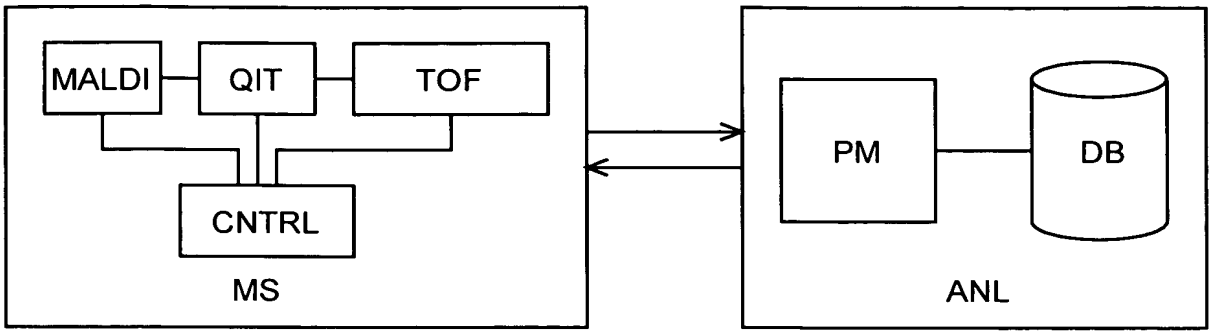

MALDI
QIT
TOF
CNTRL
MS
PM
DB
ANL

Fig. 2

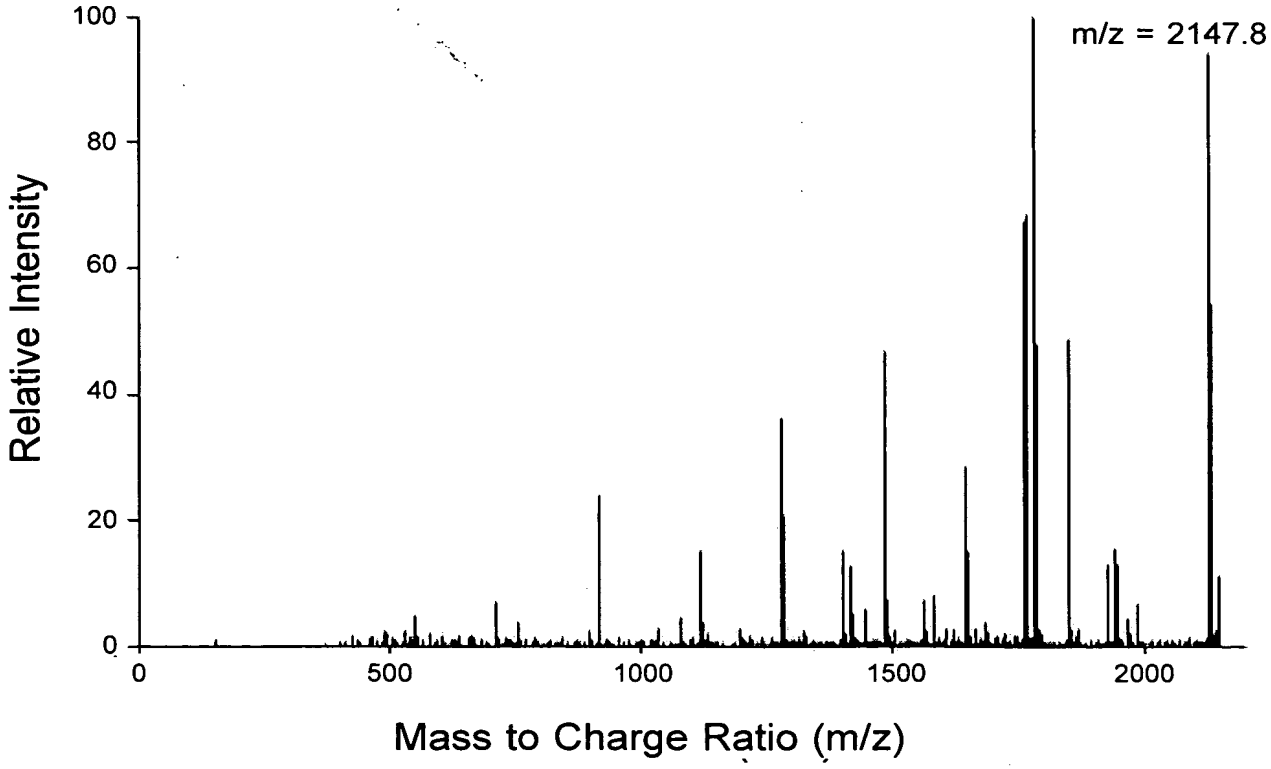
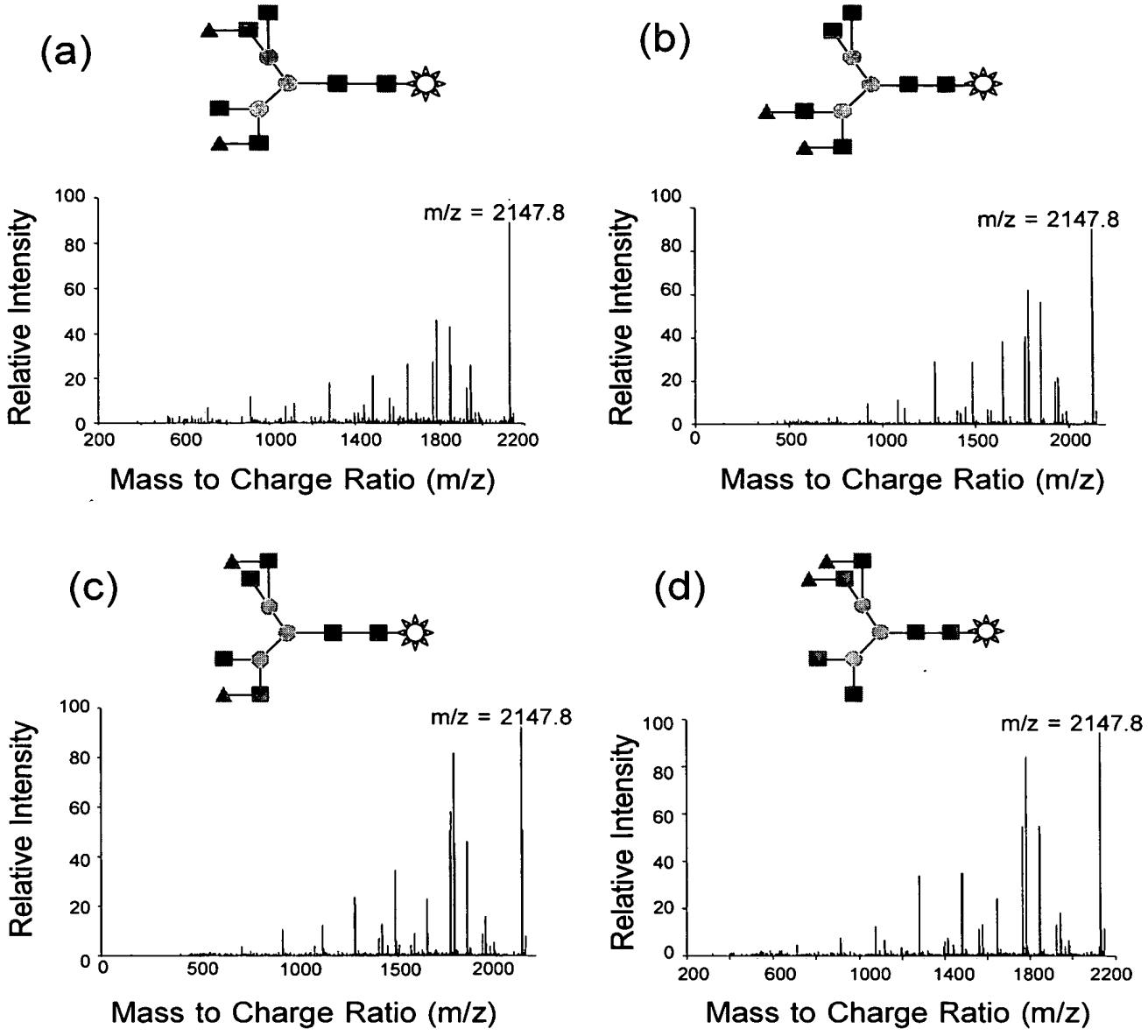
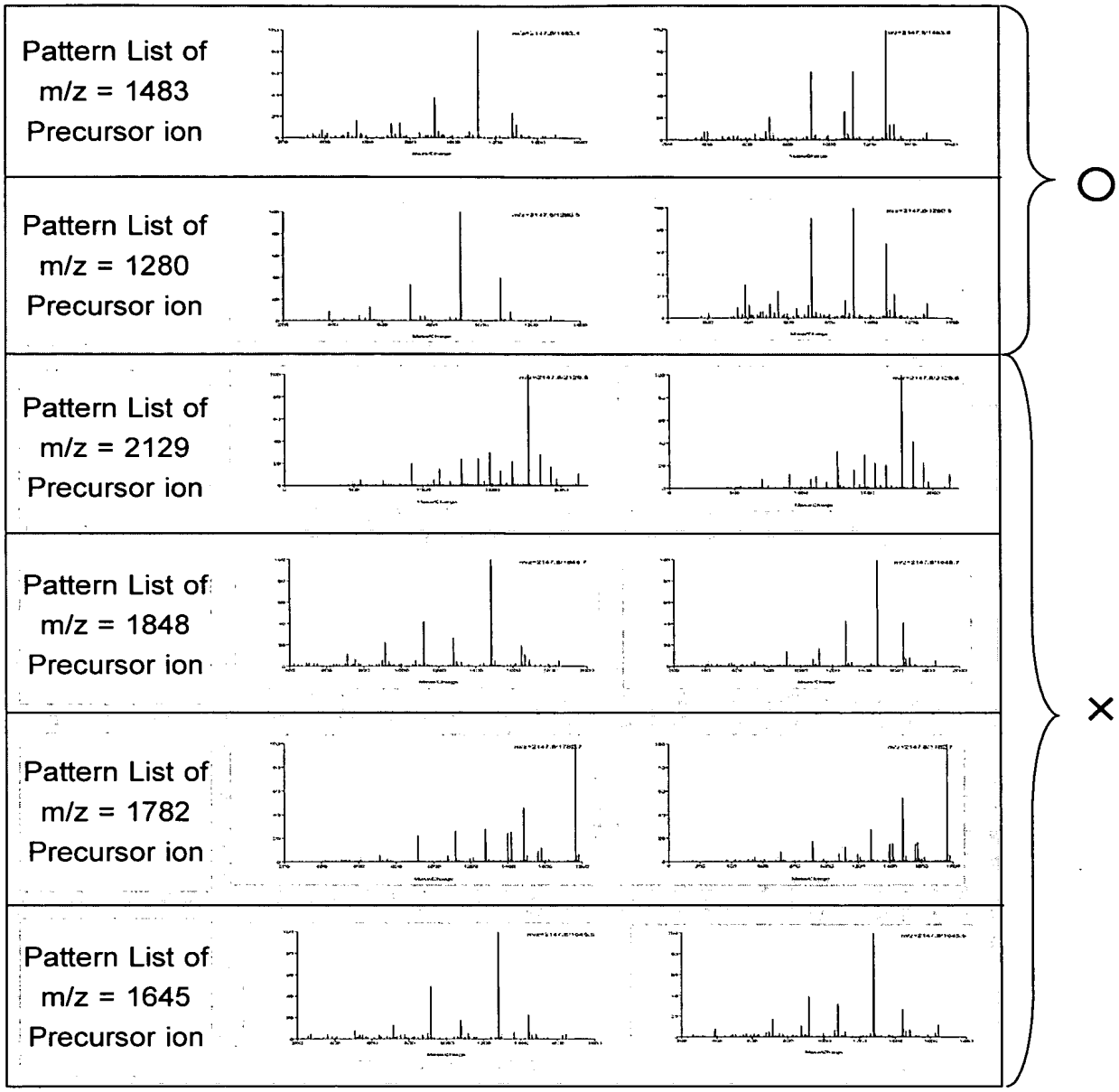

m/z = 2147.8
Relative Intensity
100
80
60
40
20
0
0
500
1000
1500
2000
Mass to Charge Ratio (m/z)

Fig. 3



Fragment Pattern	Similarity Index S((1/D) * 1E+7)	
	S1	S2
(a)	655.813	657.606
(b)	1535.890	1539.660
(c)	4570.276	4623.254
(d)	3717.617	3768.091

Fig. 4



Precursor Ion	Similarity Index S((1/D) * 1E+7)		Order
	S1	S2	
m/z=1483	1165.564	1149.987	2
m/z=1280	1140.334	1126.347	1
m/z=2129	9159.474	9079.574	-
m/z=1848	3039.331	2810.509	-
m/z=1782	7898.673	8011.952	-
m/z=1645	2881.634	2714.678	-

Fig. 5

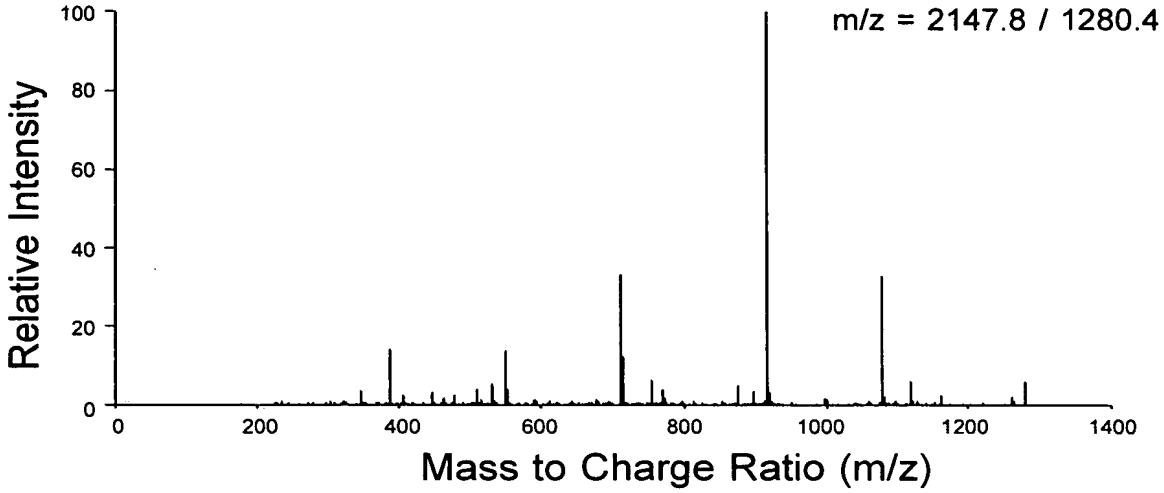
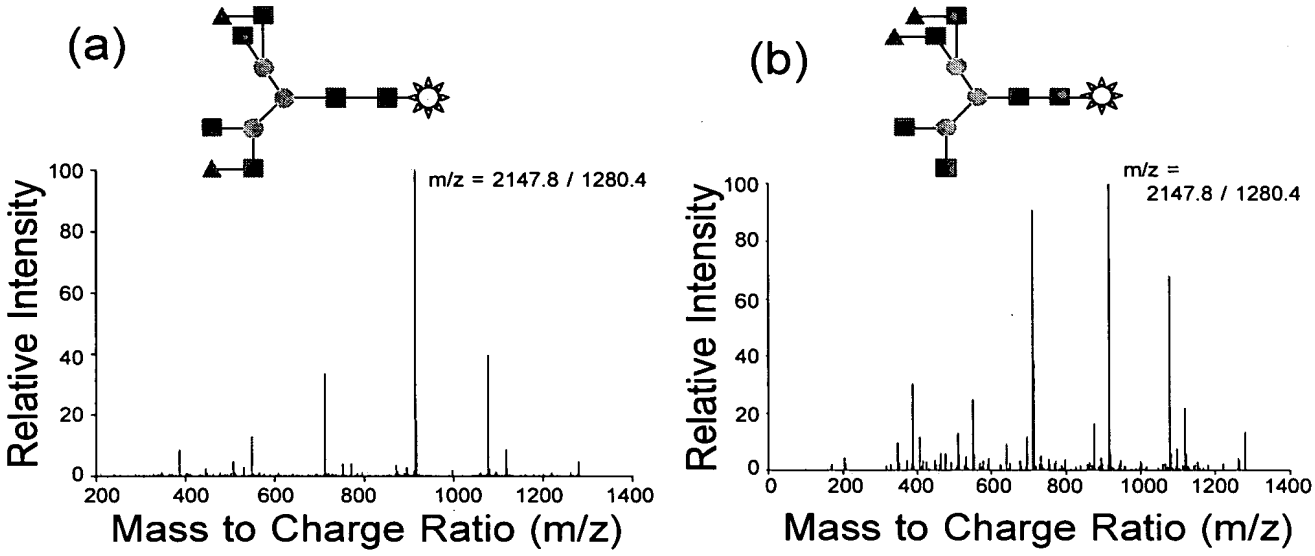
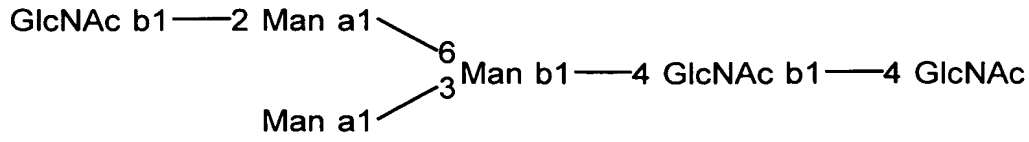


Fig. 6

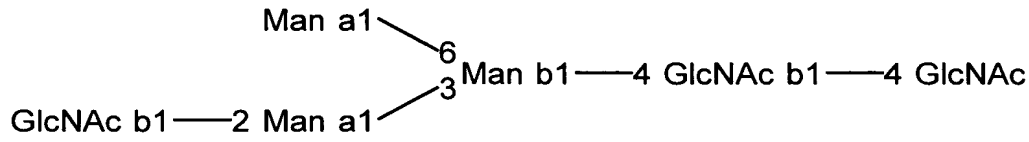


Fragment Pattern	Similarity Index S((1/D) * 1E+7)		
	S1	S2	
(a)	45166.527	45592.317	○
(b)	1158.701	1138.003	×

Fig. 7



(a) ONA−00001a(100.1)

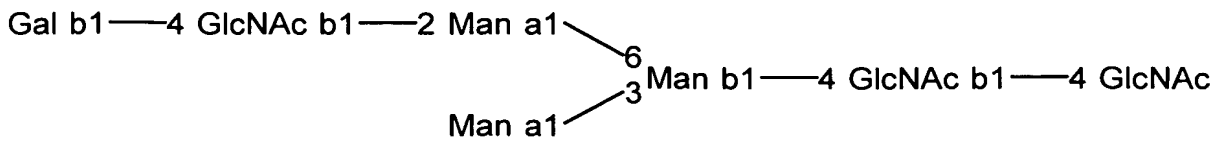


(b) ONA−00001b(100.2)

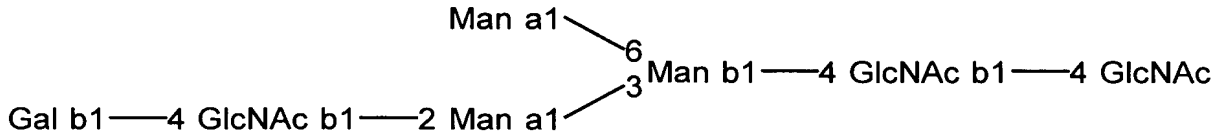
Fig. 8

Measured Sample	pre-cursor ion	MS^n	Dissimilarity between Same Samples		Peak List of Lowest Dissimilarity among Different Structures	Dissimilarity between Isomers	
ONA-00001a(100.1)	1214	2	102.8163667	102.8163667	100.2PA-MS2-1214-1.txt	100.8827	100.9693
ONA-00001a(100.1)	915	3	156.28585	156.28585	100.2PA-MS3-915-1.txt	287.2622	297.0102
ONA-00001a(100.1)	1196	3	218.16315	218.16315	100.2PA-MS3-1196-1.txt	424.273	433.6466
ONA-00001b(100.2)	1214	2	87.27248333	87.27248333	100.1PA-MS2-1214-3.txt	100.319	100.8947
ONA-00001b(100.2)	915	3	297.8943833	297.8943833	100.1PA-MS3-915-3.txt	297.0102	287.2622
ONA-00001b(100.2)	1196	3	133.9454	133.9454	100.1PA-MS3-1196-1.txt	433.6466	424.273

Fig. 9



(c) ONG—00001c(100.3)

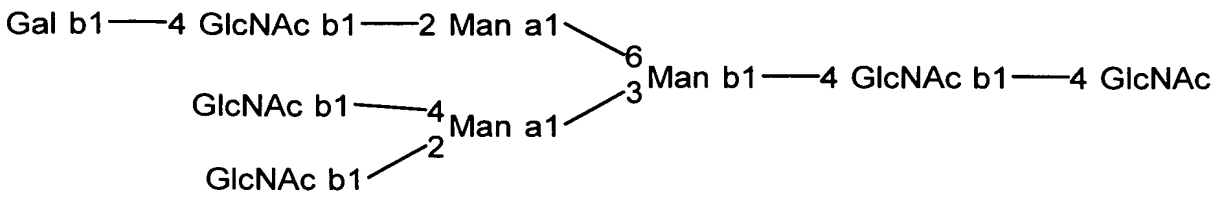


(d) ONG—00001d(100.4)

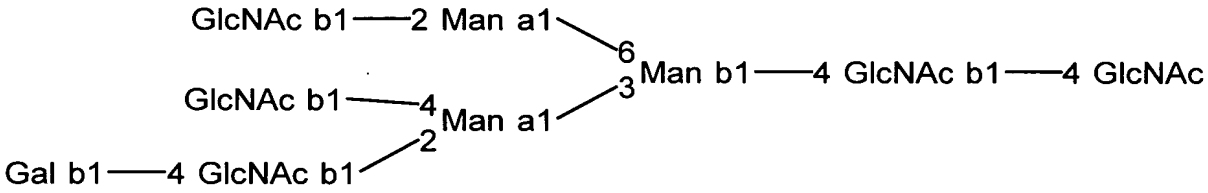
Fig. 10

Measured Sample	pre-cursor ion	MS^n	Dissimilarity between Same Samples		Peak List of Lowest Dissimilarity among Different Structures	Dissimilarity between Isomers	
ONG-00001c(100.3)	1376	2	119.2696	119.2696	100.4PA-MS2-1376-1.txt	216.5253	216.1344
ONG-00001c(100.3)	1077	3	38.76568333	38.76568333	100.1PA-MS3-915-2.txt	396.4621	467.2018
ONG-00001c(100.3)	1358	3	452.1632167	452.1632167	100.4PA-MS3-1358-3.txt	2720.1907	2722.5196
ONG-00001d(100.4)	1376	2	61.62873333	61.62873333	100.3PA-MS2-1376-2.txt	216.1344	216.5253
ONG-00001d(100.4)	1077	3	56.1829	56.1829	100.3PA-MS3-1077-1.txt	594.9353	593.819
ONG-00001d(100.4)	1358	3	207.8533167	207.8533167	100.3PA-MS3-1358-2.txt	2722.5196	2720.1907

Fig. 11



(e) ONG−00001e(310.2)

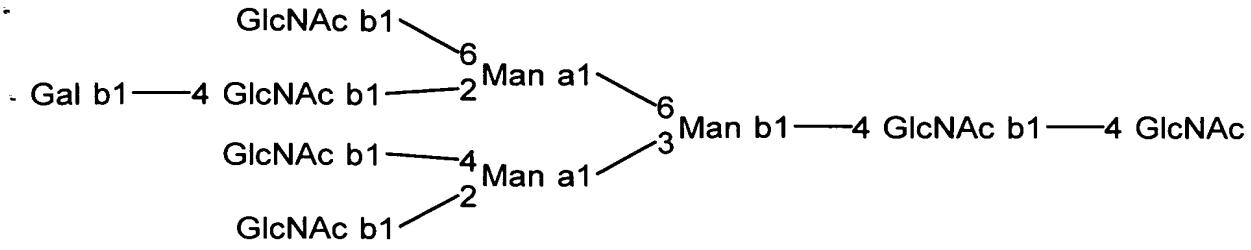


(f) ONG−00001f(310.3)

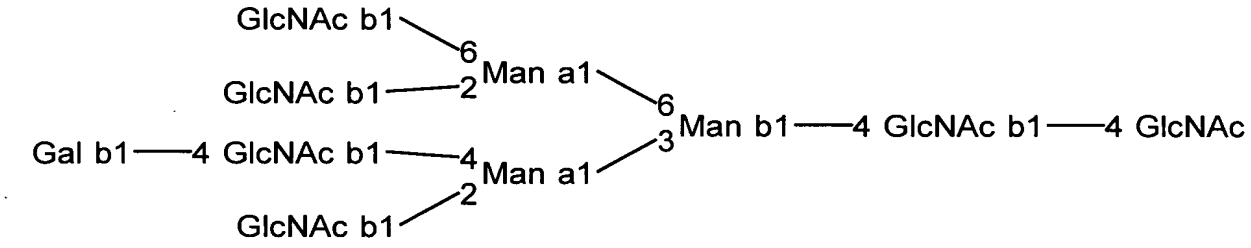
Fig. 12

Measured Sample	pre-cursor ion	MS^n	Dissimilarity between Same Samples		Peak List of Lowest Dissimilarity among Different Structures	Dissimilarity between Isomers	
ONG-00001e(310.2)	1928	2	312.2041667	312.2041667	310.3PA-MS2-1928-1.txt	160.0158	155.7346
ONG-00001e(310.2)	1280	3	655.3959833	655.3959833	310.3PA-MS3-1280-1.txt	1596.9166	1523.2752
ONG-00001e(310.2)	1483	3	174.4776167	174.4776167	310.3PA-MS3-1483-2.txt	119.2134	114.7385
ONG-00001f(310.3)	1928	2	205.0538167	205.0538167	310.2PA-MS2-1928-3.txt	155.7346	160.0158
ONG-00001f(310.3)	1280	3	290.52645	290.52645	100.2PA-MS3-1196-2.txt	1116.8702	1120.5336
ONG-00001f(310.3)	1483	3	327.5316067	327.5316067	310.2PA-MS3-1483-2.txt	114.7385	119.2134

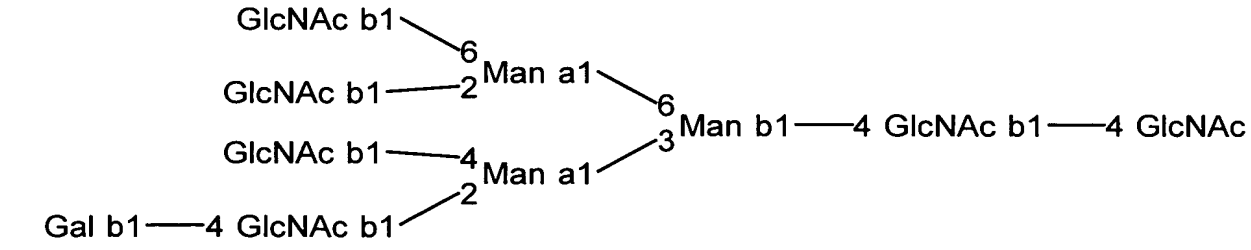
Fig. 13



(a) ONG—000020(400.2)



(b) ONG—000021(400.3)

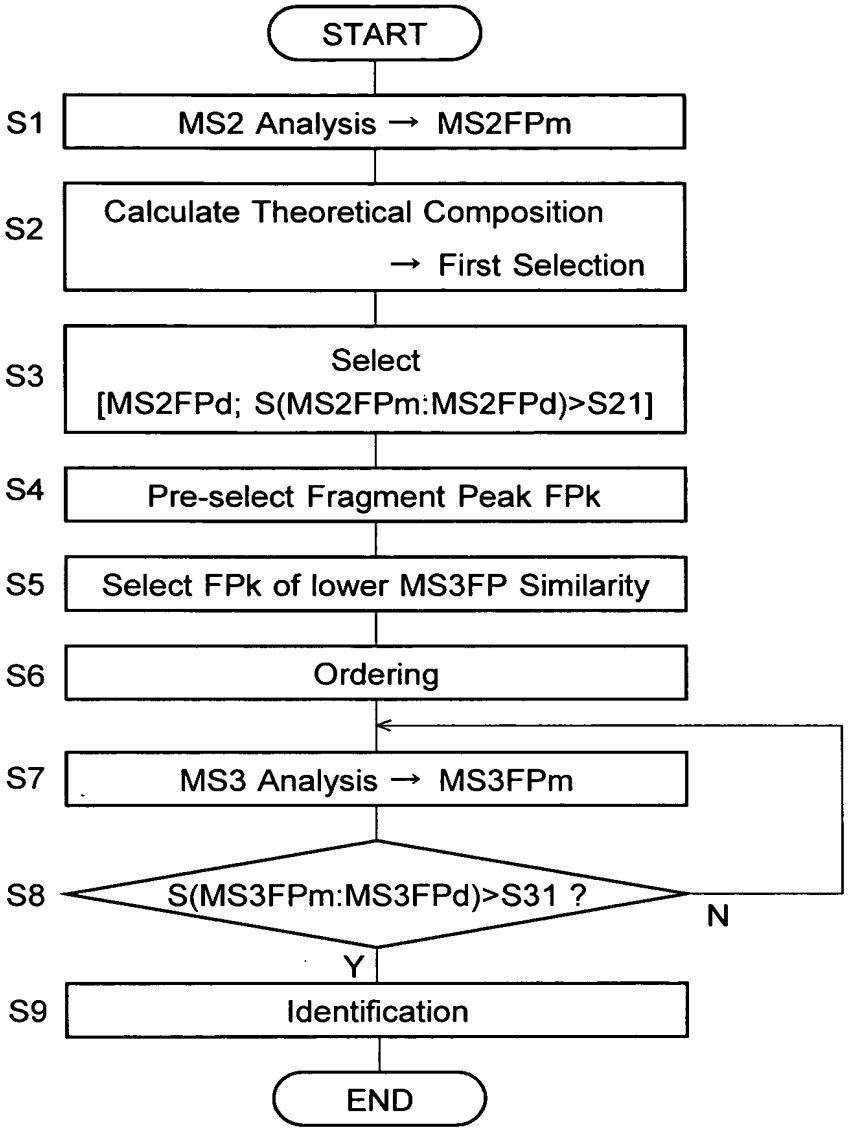


(c) ONG—000022(400.5)

Fig. 14

Measured Sample	pre-cursor ion	MS^n	Dissimilarity between Same Samples		Peak List of Lowest Dissimilarity among Different Structures	Dissimilarity between Isomers	
ONG-000020(400.2)	1985	2	858.4422167	858.4422167	400.5PA-MS2-1985-2.txt	1864.9315	1859.783
ONG-000020(400.2)	1321	3	91.71695	91.71695	400.3PA-MS3-1321-3.txt	78.5283	72.082
ONG-000020(400.2)	1483	3	411.9361833	411.9361833	400.5PA-MS3-1483-3.txt	239.7108	267.7883
ONG-000020(400.2)	1602	3	969.9182	969.9182	400.5PA-MS3-1602-3.txt	1103.5193	1101.6843
ONG-000020(400.2)	1686	3	533.01535	533.01535	400.5PA-MS3-1686-2.txt	3936.2343	3955.8892
ONG-000020(400.2)	1764	3	378.8141	378.8141	400.5PA-MS3-1764-2.txt	4367.2301	4411.4233
ONG-000020(400.2)	1967	3	281.67725	281.67725	No Spectrum under 10000		
ONG-000021(400.3)	1985	2	455.7612167	455.7612167	400.5PA-MS2-1985-1.txt	257.98	250.1656
ONG-000021(400.3)	1321	3	123.00805	123.00805	400.5PA-MS3-1321-1.txt	42.8943	45.8055
ONG-000021(400.3)	1483	3	256.8724167	256.8724167	310.2PA-MS3-1483-3.txt	1801.5073	1739.7947
ONG-000021(400.3)	1602	3	338.1913972	338.1913972	400.5PA-MS3-1602-1.txt	353.2306	352.4087
ONG-000021(400.3)	1686	3	307.1847167	307.1847167	400.5PA-MS3-1686-3.txt	3834.4255	3836.0349
ONG-000021(400.3)	1764	3	813.7935	813.7935	400.5PA-MS3-1764-1.txt	5369.3515	5352.7886
ONG-000021(400.3)	1967	3	800.1308	800.1308	400.5PA-MS3-1967-2.txt	6323.3696	6343.6005
ONG-000022(400.5)	1985	2	283.9350667	283.9350667	400.3PA-MS2-1985-2.txt	250.1656	257.98
ONG-000022(400.5)	1321	3	106.6899667	106.6899667	400.3PA-MS3-1321-2.txt	45.8055	42.8943
ONG-000022(400.5)	1483	3	256.8044	256.8044	400.2PA-MS3-1483-3.txt	267.7883	239.7108
ONG-000022(400.5)	1602	3	700.73915	700.73915	400.3PA-MS3-1602-3.txt	352.4087	353.2306
ONG-000022(400.5)	1686	3	720.2411167	720.2411167	400.3PA-MS3-1686-1.txt	3836.0349	3834.4255
ONG-000022(400.5)	1764	3	1014.059233	1014.059233	400.2PA-MS3-1764-2.txt	4411.4233	4367.2301
ONG-000022(400.5)	1967	3	513.7448222	513.7448222	400.3PA-MS3-1967-3.txt	6343.6005	6323.3696

Fig. 15


START
S1
MS2 Analysis → MS2FPm
S2
Calculate Theoretical Composition
→ First Selection
S3
Select
[MS2FPd; S(MS2FPm:MS2FPd)>S21]
S4
Pre-select Fragment Peak FPk
S5
Select FPk of lower MS3FP Similarity
S6
Ordering
S7
MS3 Analysis → MS3FPm
S8
S(MS3FPm:MS3FPd)>S31 ?
N
Y
S9
Identification
END